

L-Proline, N-(3-bromobenzoyl)-, isohexyl ester

Inchi: InChI=1S/C18H24BrNO3/c1-13(2)6-5-11-23-18(22)16-9-4-10-20(16)17(21)14-7-3-8-15(1)
InchiKey: VWZCPNCBTSIMIQ-UHFFFAOYSA-N
Formula: C18H24BrNO3
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 382.29

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.17 | | Crippen Method |
| logp | 4.033 | | Crippen Method |
| mcvol | 266.350 | ml/mol | McGowan Method |
| rinpol | 2663.00 | | NIST Webbook |
| rinpol | 2663.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346141&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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